JOURNAL OF MOLECULAR STRUCTURE, VOLUME 224 (1990)

AUTHOR INDEX

Abliz, Z., 313
Aboab, B., 89
Aoki, J., 313
Atalla, R.H., 385

Bailey, G.F., 245
Baranov, V.I., 45
Becucci, M., 471
Bock, C.W., 89
Bolton, B.A., 245
Borionetti, G., 425
Bowman, J.M., 133

Califano, S., 471
Campani, E., 271
Castellucci, E., 471
Castiglioni, C., 445
Cavalli, R., 271
Cuniberti, C., 271

De la Cruz, C., 141
Dellepiane, G., 271
Devlin, J.P., 33
Dowrey, A.E., 265
Dows, D.A., 471
Durig, J.R., 323

Fox, K., 1
Freedman, T.B., 121
Fukuhara, K., 203

Golden, D.M., 357
Gorini, G., 271
Gough, K.M., 73
Gribov, L.A., 45
Gussoni, M., 445

Hadži, D., 285
Hamada, Y., 345
Hardin, J.A., 323
Hester, R.E., 113

Ikeda, K., 203
Iwashima, S., 313

Jennings, D.E., 1

Kan, T., 313
Kindness, A., 363
Kint, S., 245
Krimm, S., 7
Kubulat, K., 225
Kuchitsu, K., 345

Luck, W.A.P., 175, 185

Machida, K., 163
Marcott, C., 265
Masetti, G., 271
Matsunaga, S., 313
Matsuura, H., 203
Matsuzawa, T., 345
Mavri, J., 285
McEwen, A.B., 357
McKean, D.C., 363
Mercurio, J.P., 303
Murphy, W.F., 73

Nafie, L.A., 121
Nishimura, M., 313
Noda, I., 265
Noma, H., 163

Parthenopoulos, D.A., 297
Peil, S., 175, 185
Person, W.B., 225
Pradeep, T., 21

Raam Somayajulu, G., 259
Ramos, M.N., 445
Rao, C.N.R., 21
Redington, R.L., 89
Rentzepis, P.M., 297
Rui, M., 445

Sato, M., 313
Schafer, P., 133
Scherer, J.R., 245
Schriver, A., 185
Schriver, L., 185
Sheppard, N., 141
Stewart, D., 363

Tanaka, R., 313
Tolley, C.L., 323
Tsuboi, M., 345
Turrell, G., 303
Turrell, S., 303

Ueda, T., 313
Umapathy, S., 113

Van Tien, N., 471

Wells, Jr., H.A., 385
Wiberg, K.B., 61

Yahia, Z., 303
Yamanouchi, K., 345

Zannoni, G., 425
Zerbi, G., 425, 445
Zhao, W.-Y., 7
Zwolinski, B.J., 259

JOURNAL OF MOLECULAR STRUCTURE, VOLUME 224 (1990)

SUBJECT INDEX

Acetonitrile,
IR studies of van der Waals interactions on perfluoro-t-butyl alcohol OH. Part II. Complexes with acetonitrile, 185
Acetylene,
The Raman scattering intensity parameters of acetylene, 73
Allyllamine,
Rotational isomerism of allylamine as studied by gas electron diffraction: a joint analysis with rotational constants and SCF MO calculation, 345
1-Azabenzanthrone,
Structure determination by MS, NMR and UV spectra of bromo and nitro derivatives of 1-azabenzanthrone, 313
Azines,
Azines. Effect of basis set on calculated vibrational frequencies, infrared intensities and Raman intensities, 61

Benzylimidazolidine,
Tautomerism, protonation, and interaction with formiate, of phenyliminoimidazoline and benzylimidazolidine: AM1 and ab initio 4-31G calculations, 285
Bipolarons,
Raman spectroscopic studies of polypyrrole on colloidal TiO_2: evidence for bipolarons, 113

t-C_4H_9,
Reaction of t-C_4H_9. with HI: possible negative activation energies, 357
β-Carotene,
Polarized Raman spectra of oriented all-*trans*-β-carotene in polyethylene films, 271
CH stretching bands,
Infrared intensities of CH stretching bands in partially deuterated compounds, and effects of conformation and substitution, 363
Circular dichroism,
Electronic current models of vibrational circular dichroism, 121
Clusters,
A review of νCO bond-stretching wavenumbers for CO ligands in metal coordination compounds or clusters with emphasis on the less common types of metal/CO bonding patterns, and of the relationship between νCO and the internuclear distance, νCO 141
Colloidal TiO_2,
Raman spectroscopic studies of polypyrrole on colloidal TiO_2: evidence for bipolarons, 113
Coordination compounds,
A review of νCO bond-stretching wavenumbers for CO ligands in metal coordination compounds or clusters with emphasis on the less common types of metal/CO bonding patterns, and of the relationship between νCO and the internuclear distance, 141
18-Crown-6,
Normal coordinate analysis and force-field of 18-crown-6, 203

Deuterated compounds,
Infrared intensities of CH stretching bands in partially deuterated compounds, and effects of conformation and substitution, 363
Diatomic molecules,
Spectroscopic studies of methane in collisions with rare gas atoms and diatomic molecules, 1
Dichloroacetone,
Conformational analysis, barriers to internal rotation, ab initio calculations and vibrational assignment for 1,1-dichloroacetone, 323
Dihydroxycarbene,

MO study of the monomer and adducts of dihydroxycarbene, 89
Disordered polymers,
Lattice dynamics and vibrational spectra of conformationally disordered polymers: poly(vinylidene fluoride), 425
Disulfide group,
Vibrational studies of the disulfide group in proteins. Part II. Ab initio force fields and normal mode frequencies of dimethyl, methylethyl, and diethyl disulfides, 7

Floppy molecules,
A new functional form for global potentials of floppy molecules, 133
Formiate,
Tautomerism, protonation, and interaction with formiate, of phenyliminoimidazoline and benzylimidazolidine: AM1 and ab initio 4-31G calculations, 285
Fulgide,
Transient spectroscopy of a photochromic fulgide, 297

Galactose,
An investigation of the vibrational spectra of glucose, galactose and mannose, 385
Global potentials,
A new functional form for global potentials of floppy molecules, 133
Glucose,
An investigation of the vibrational spectra of glucose, galactose and mannose, 385

H_2O,
Interpretation of infrared intensities. Part II. An intensity analysis, with applications to H_2O, 225
Vibrational modes of amorphous ice: bending mode frequencies for isotopically decoupled H_2O and HOD at 90 K, 33
Hexaborides,
Infrared and Raman spectra of hexaborides: force-field calculations and isotopic effects, 303
Humidity-dependent phase transitions,
Raman spectra of hydrated phospholipid bilayers. Part 1. Measurement of humidity-dependent phase transitions, 245
Hydrogen bonded complexes,
Electronic transitions of hydrogen bonded complexes: an electron energy loss spectroscopic study, 21

Ice,
Vibrational modes of amorphous ice: bending mode frequencies for isotopically decoupled H_2O and HOD at 90 K, 33
Infrared intensities,
Infrared intensities: from intensity parameters to an overall understanding of the spectrum, 445
Intensity analysis,
Interpretation of infrared intensities. Part II. An intensity analysis, with applications to H_2O, 225
Intensity parameters,
Infrared intensities: from intensity parameters to an overall understanding of the spectrum, 445
The Raman scattering intensity parameters of acetylene, 73

Large molecules,
A non-adiabatic semi-empirical method for calculating the electron-vibrational spectra of large molecules. A possible approach for future studies, 45
Lattice dynamics,
Lattice dynamics and vibrational spectra of conformationally disordered polymers: poly(vinylidene fluoride), 425
Lattice phonons,
High resolution Raman measurements of the temperature variation of the bandwidth of some lattice phonons and of one internal vibron of α-oxalic acid, 471

Mannose,
An investigation of the vibrational spectra of glucose, galactose and mannose, 385
Metal/CO bonding patterns,
A review of νCO-stretching wavenumbers for CO ligands in metal coordination compounds or clusters with emphasis on the less common types of metal/CO bonding patterns, and of the relationship between νCO and the internuclear distance, νCO 141
Methane,
Spectroscopic studies of methane in colli-

sions with rare gas atoms and diatomic molecules, 1

Negative activation energies,
Reaction of t-C_4H_9. with HI: possible negative activation energies, 357
Non-adiabatic semi-empirical method,
A non-adiabatic semi-empirical method for calculating the electron-vibrational spectra of large molecules. A possible approach for future studies, 45

OH,
IR studies of van der Waals interactions on perfluoro-t-butyl alcohol OH. Part I. Environment effects on monomeric OH and self-associates, 175
IR studies of van der Waals interactions on perfluoro-t-butyl alcohol OH. Part II. Complexes with acetonitrile, 185
Oxalic acid,
High resolution Raman measurements of the temperature variation of the bandwidth of some lattice phonons and of one internal vibron of α-oxalic acid, 471

Perfluoro-t-butyl alcohol,
IR studies of van der Waals interactions on perfluoro-t-butyl alcohol OH. Part I. Environment effects on monomeric OH and self-associates, 175
IR studies of van der Waals interactions on perfluoro-t-butyl alcohol OH. Part II. Complexes with acetonitrile, 185
Phenyliminoimidazoline,
Tautomerism, protonation, and interaction with formiate, of phenyliminoimidazoline and benzylimidazolidine: AM1 and ab initio 4-31G calculations, 285
Phospholipid bilayers,
Raman spectra of hydrated phospholipid bilayers. Part 1. Measurement of humidity-dependent phase transitions, 245
Photochromic,
Transient spectroscopy of a photochromic fulgide, 297
Poly(vinylidene fluoride),
Lattice dynamics and vibrational spectra of conformationally disordered polymers: poly(vinylidene fluoride), 425
Polyethylene,
Dynamic infrared linear dichroism study of high-density and low-density polyethylene near the β-transition temperature, 265
Polyethylene films,
Polarized Raman spectra of oriented all-*trans*-β-carotene in polyethylene films, 271
Polypyrrole,
Raman spectroscopic studies of polypyrrole on colloidal TiO_2: evidence for bipolarons, 113
Proteins,
Vibrational studies of the disulfide group in proteins. Part II. Ab initio force fields and normal mode frequencies of dimethyl, methylethyl, and diethyl disulfides, 7

Rotational constants,
Rotational isomerism of allylamine as studied by gas electron diffraction: a joint analysis with rotational constants and SCF MO calculation, 345

SCF MO calculations,
Rotational isomerism of allylamine as studied by gas electron diffraction: a joint analysis with rotational constants and SCF MO calculation, 345
Sodium formate crystal,
Polarized Raman intensities of sodium formate crystal and its non-cylindrical electrooptical parameters, 163

Trigonal additivity,
The concept of trigonal additivity, 259